

# Sorption, Structure and Dynamics of CO<sub>2</sub> and Ethane in Silicalite at High Pressure: A Combined Monte Carlo and Molecular Dynamics Simulation Study

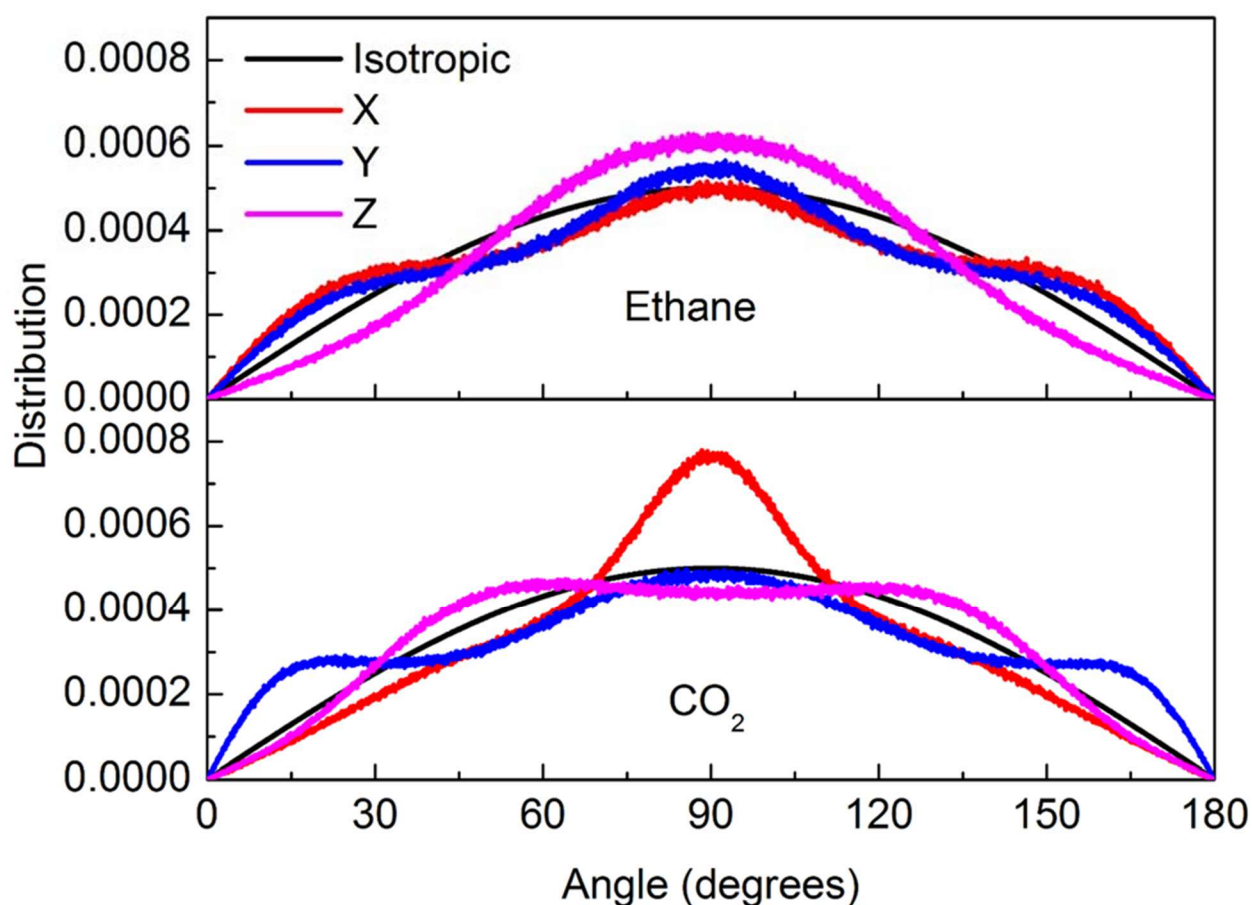
Siddharth Gautam \*, Tingting Liu and David Cole

School of Earth Sciences, The Ohio State University, Columbus, OH 43210, USA;

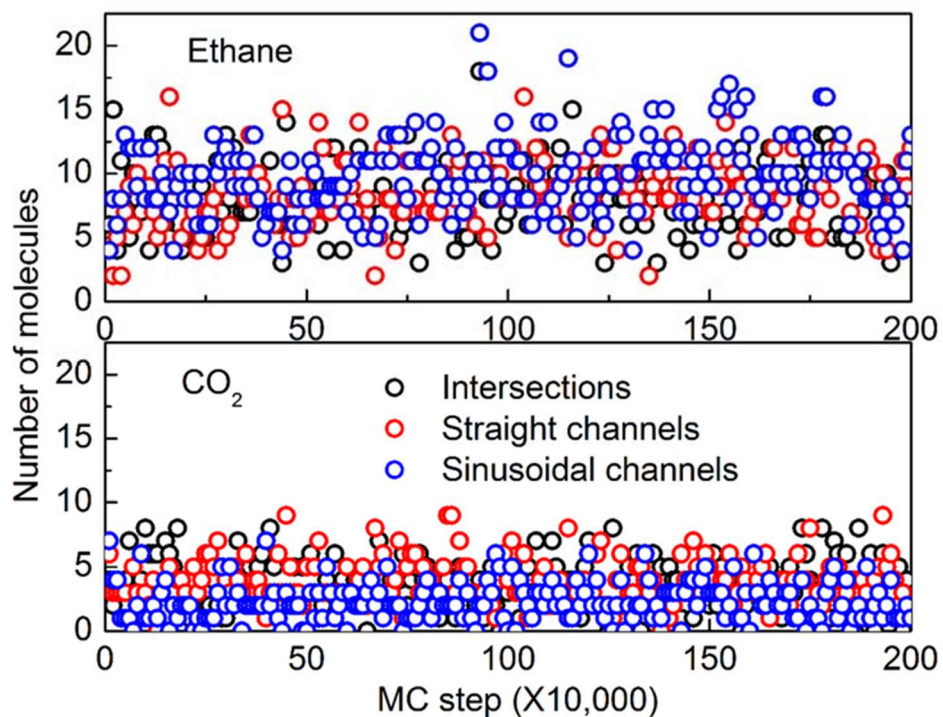
liu.2189@osu.edu (T.L.); cole.618@osu.edu (D.C.)

\* Correspondence: gautam.25@osu.edu; Tel.: +01-614-292-7365

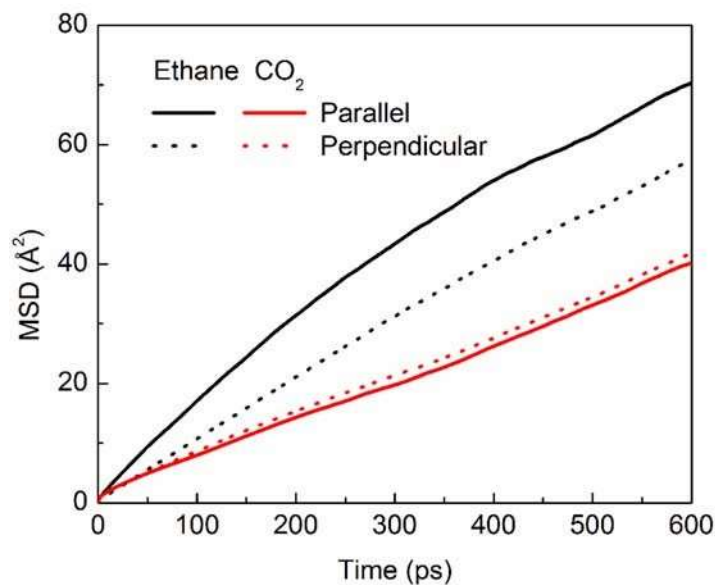
## Supplementary Materials



**Figure S1.** Orientational distribution functions of ethane and CO<sub>2</sub> in all pores of silicalite with respect to the Cartesian axes X (red), Y (blue) and Z (magenta). Distribution expected in case of an isotropic system is also included for reference as a black curve.



**Figure S2.** Distribution of ethane and CO<sub>2</sub> in straight and sinusoidal channels and their intersections at 0.05 bar. Even though the total number of sorbed molecules at this pressure is low, all types of pores get populated.



**Figure S3.** MSD of ethane and CO<sub>2</sub> parallel and perpendicular to the molecular axis at 100 bar. Note that the MSD in a direction perpendicular to the molecular axis shown here has been divided by 2 for normalization. This is because, while only one direction can be parallel to the molecular axis, 2 mutually orthogonal directions can be perpendicular to the molecular axis.